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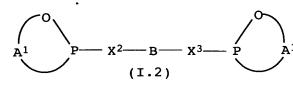
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A catalyst comprising at least one complex of a metal of transition group VIII comprising at least one monodentate, bidentate or multidentate phosphinamidite ligand of the formulae I.1, I.2 and/or I.3

 $A^{1} \qquad P \qquad X^{1}$



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 $X^1 \longrightarrow P \longrightarrow A^2 \longrightarrow B \longrightarrow A^3 \longrightarrow P \longrightarrow X$

where

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A¹ together with the phosphorus atom and the oxygen atom to which it is bound form a 5- to 8-membered heterocycle onto which one, two or three cycloalkyl, aryl and/or hetaryl groups may be fused, where the fused-on groups may each bear, independently of one another, one, two or three substituents selected from among alkyl, alkoxy, halogen, nitro, cyano, carboxyl and carboxylate,

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 A^2 and A^3 are, independently of one another, part of a heterocycle as defined for A^1 which is substituted by B,

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is a 5- to 8-membered heterocycle which contains at least one nitrogen atom bound directly to the phosphorus atom, where the heterocycle may additionally contain one or two heteroatom(s) selected from among N, O and S and/or one, two or three cycloalkyl, aryl and/or hetaryl groups may be fused onto the heterocycle, where the heterocycle and/or the fused-on groups may each bear, independently of one another, one, two or three substituents selected from among alkyl, cycloalkyl, aryl, alkoxy, cycloalkoxy, aryloxy, acyl, halogen, trifluoromethyl, nitro, cyano, carboxyl, carboxylate, alkoxycarbonyl and NE¹E², where E¹ and E² may be identical or different and are each alkyl,

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 X^2 and X^3 are, independently of one another, a heterocycle as defined for X^1 which is substituted by B,

cycloalkyl or aryl,

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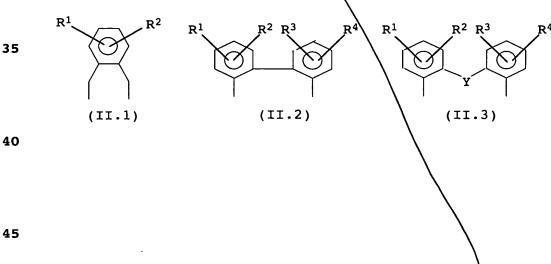
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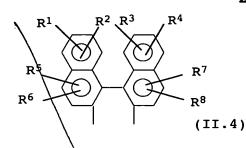
is either a carbon-carbon single bond or a divalent bridging group,

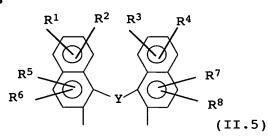
5 or salts or mixtures thereof.

- 2. A catalyst as claimed in claim 1, wherein B is a bridging group of the formula -D-, -(CO)-D-(CO)- or -(CO)-(CO)-, in which
 - is a C_1-C_{10} -alkylene bridge which may have one, two, D three or four double bonds and/or bear one, two, three or four substituents selected from among alkyl, alkoxy, halogen, \nitro, cyano, carboxyl, carboxylate, cycloalkyl and aryl, where the aryl substituent may additionally bear one, two or three substituents selected from among alkyl, alkoxy, halogen, trifluoromethyl, nitro, alkoxycarbon or cyano, and/or the alkylene bridge D may be interrupted by one, two or three nonadjacent, substituted or\unsubstituted heteroatoms, and/or the alkylene bridge\D may have one, two or three aryl and/or hetaryl groups fused onto it, where the fused-on aryl and hetaryl groups may each bear one, two or three substituents selected from among alkyl, cycloalkyl, aryl, alkoxy, cycloalkoxy aryloxy, aryl, halogen, trifluoromethyl, nitto, cyano, carboxyl, alkoxycarbonyl and NE1E2, where E1 and E2 may be identical or different and are each alkyl, cycloalkyl or aryl.

3. A catalyst as claimed in claim 2, wherein D is a radical of the formula II.1, II.2, II.3, II.4 or II.5







where

10 Y is O, S,\NR⁹, where
R⁹ is alkxl, cycloalkyl or aryl,

or Y is a C₁-C₃-alkylene bridge which may have a double bond and/or an alkyl, cycloalkyl- or aryl substituent, where the aryl substituent may bear one, two or three substituents selected from among alkyl, alkoxy, halogen, trifluoromethyl, nitro, alkoxycarbonyl and cyano,

or Y is a C_2-C_3 -alkylene bridge which is interrupted by O, S or NR⁹,

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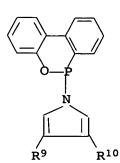
R¹, R², R³, R⁴, R⁵, R⁶, R⁷ and R⁸ are, independently of one another hydrogen, alkyl, cycloalkyl, aryl, alkoxy, halogen, trifluoromethyl, nitro, alkoxycarbonyl or cyano.

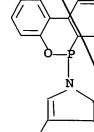
4. A catalyst as claimed in any of the preceding claims, wherein the phosphinamidite ligand is selected from among the ligands of the formulae IIIa to IIIi

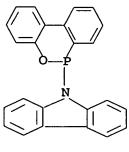
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(IIIa)

(IIIb)

(IIIC)

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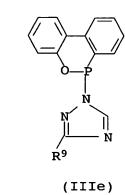
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R10

R⁹

(IIId)

(IIIg)

(IIIh)

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where

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 R^9 and R^{10} are, independently of one another, hydrogen, methyl, ethyl or trifluoromethyl,

(IIIi)

R¹¹ is hydrogen or COOC₂H₅,

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B is CH_2 , $C(CH_3)_2$, (CO)-(CO) or (CO)-D-(CQ),

where B in the formulae IIIg, IIIh and IIIi can in each case be bound in the o,o positions, m,m positions or p,p positions relative to the phosphorus atoms and

- D is a C_1-C_{10} alkylene bridge as defined in claim 2 or 3.
- 45 5. A catalyst as claimed in any of the preceding claims, wherein the metal of transition group VIII is selected from among cobalt, ruthenium, iridium, rhodium, nickel, palladium and





platinum.

- 6. A catalyst as claimed in any of the preceding claims which further comprises at least one further ligand selected from among halides, amines, carboxylates, acetylacetonate, arylsulfonates or alkylsulfonates, hydride, CO, olefins, dienes, cycloolefins, nitriles, N-containing heterocycles, aromatics and heteroaromatics, ethers, PF₃ and monodentate, bidentate and multidentate phosphine, phosphinite,
 phosphonite and phosphite ligands.
 - 7. A process for the hydroformylation of compounds which contain at least one ethylenically unsaturated double bond by reaction with carbon monoxide and hydrogen in the presence of a hydroformylation catalyst, wherein the hydroformylation catalyst used is a catalyst as claimed in any of claims 1 to 6.
- 8. A process for the hydrocyanation of compounds containing at least one ethylenically unsaturated double bond by reaction with hydrogen cyanide in the presence of a hydrocyanation catalyst, wherein the hydrocyanation catalyst used is a catalyst as claimed in any of claims 1 to 6.
- 25 9. A process as claimed in claim 7 or 8, wherein the hydroformylation catalyst or the hydrocyanation catalyst is prepared in situ by reacting at least one phosphinamidite ligand as defined in any of claims 1 to 6, a compound or a complex of a metal of transition group VIII and, if desired, an activator in an inert solvent under the hydroformylation conditions or the hydrocyanation conditions.
 - 10. The use of a catalyst comprising a phosphinamidite ligand as claimed in any of claims 1 to 6 for the hydroformylation or hydrocyanation of compounds having at least one ethylenically unsaturated double bond.

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Catalyst comprising a complex of a metal of transition group VIII based on a phosphinamidite ligand

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Abstract

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A catalyst comprising at least one complex of a metal of transition group VIII comprising at least one monodentate, bidentate or multidentate phosphinamidite ligand in which the phosphorus atom and the oxygen atom of the phosphinamidite group 10 form part of a 5- to 8-membered heterocycle can be used for the hydroformylation and hydrocyanation of compounds containing at least one ethylenically unsaturated double bond.

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